

Semi-classical study of the Quantum Hall conductivity.

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The semi-classical study of the integer Quantum Hall conductivity is investigated for electrons in a bi-periodic potential $V(x, y)$. The Hall conductivity is due to the tunnelling effect and we concentrate our study to potentials having three wells in a periodic cell. A non-zero topological conductivity requires special conditions for the positions, and shapes of the wells. The results are derived analytically and well confirmed by numerical calculations.

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I. INTRODUCTION

Some physical phenomenon happen to be expressible from topological properties of specific models. The integer Hall conductivity is one of them [9], [27]. In a simple model of non-interacting electrons moving in a two-dimensional periodic potential $V(x, y)$ subject to a uniform perpendicular magnetic field B_z and a low electric field E_y , the Hall conductivity σ_{xy} of a given filled Landau electronic band turns out to be proportional to an integer C :

$$\sigma_{xy} = \frac{e^2}{h} C$$

C is the Chern index of the band, describing the topology of its fiber bundle structure [25], [15], [9], [8].

For a better understanding of this phenomenon, and to bring out the conditions of possible experimental measures, we investigate in this paper the value of C as a function of the potential V . This is done by semi-classical methods, and the tunnelling effect appears to be the fundamental mechanism for a non-zero conductivity.

In the limit of high magnetic field B_z , the above model is mapped onto the well-known Harper model, by means of the Peierls substitution: the potential V is considered as a perturbation of the cyclotron motion, and the averaging method of mechanics gives an effective Hamiltonian equal to the average of V on the cyclotron circles. We neglect the coupling between the Landau bands [26]. For a high magnetic field, (hence for a small cyclotron radius,) this transformation gives an effective Hamiltonian $H_{eff}(q, p) \sim V(q, p)$, which is biperiodic in position and momentum (the phase space is a 2D torus), and an effective Planck constant $\hbar_{eff} = \hbar c / (eB)$. In this approximation, trajectories are the levels lines of $H_{eff} \sim V$. Furthermore, the expression of \hbar_{eff} shows that the high magnetic field regime corresponds to the semi-classical limit. This model will be the starting point of our study in the next section.

Quantum mechanics on the torus has been extensively used as a convenient framework to study basic properties of the semi-classical limit like quantum chaos ([18], [19], [20], [5]), or the tunnelling effect ([31,32], [3]). For this purpose, a convenient tool is the Bargmann and Husimi representation which maps a quantum state to a function on the phase space. These representations are constructed with coherent states and will be recalled in section 3.

The new results presented in this paper are the conditions under which the tunnelling effect between three different wells can be responsible for a non-zero Hall conductivity. The conditions will be expressed by specifying the special positions the three wells must have inside a periodic cell.

It is worth mentioning that due to its topological aspect, it is natural to study the Chern index values in a generic

situation, because topological properties are robust against perturbations. Secondly, in the generic ensemble of Hamiltonian under study, the integer values of the Chern indices are characterized by the position of the boundary where their value changes by one unit. These boundaries turn out to correspond to degeneracies in the spectrum [2]. We are therefore brought to study the generic location of these degeneracies, in the space of Hamiltonians. This is done in section 5 and 6.

Under reasonable assumptions on the tunnelling interaction in phase space, we find that the boundary of constant Chern index domain form ellipses in any generic two-dimensional subspace of the Hamiltonian's space. These analytical results are well confirmed by numerical calculations in section 7.

These results extend previous work by the first author for the Hall conductivity resulting from the tunneling effect between two wells in a given periodic cell ([10], [11]). Although the methods looks similar, calculations and results are quite different.

II. QUANTUM MECHANICS ON THE TORUS

A. Classical dynamics on the torus

Let us consider a one-degree of freedom Hamiltonian (hence an integrable dynamics), periodic both in position q and momentum p , with respective periods Q and P :

$$H(q, p) = H(q + Q, p) = H(q, p + P) \quad (1)$$

The function $H(q, p)$ can be decomposed into its Fourier series:

$$H(q, p) = \sum_{n_1, n_2 \in \mathbb{Z}^2} c_{n_1, n_2} \exp(i2\pi n_1 \frac{q}{Q}) \exp(i2\pi n_2 \frac{p}{P}) \quad (2)$$

This decomposition will be used for numerical computations, but is not essential for the theoritical part of this work.

Since H is a real valued function, the complex coefficients c_{n_1, n_2} must satisfy:

$$c_{n_1, n_2} = \bar{c}_{-n_1, -n_2} \in \mathbb{C}, \quad (n_1, n_2) \in \mathbb{Z}^2$$

The trajectories $q(t), p(t)$ evolve on the plane, but because of periodicity, they can be considered as trajectories on the Torus T_{qp} , obtained by identifying the opposite sides of the cell $[0, Q] \times [0, P]$.

For example, the trajectories of the Harper Hamiltonian

$$H(q, p) = -\cos(2\pi \frac{q}{Q}) - \frac{1}{2} \cos(2\pi \frac{p}{P}) \quad (3)$$

are displayed in figure 1, p. 2. Some energy levels are contractibles, others are not.

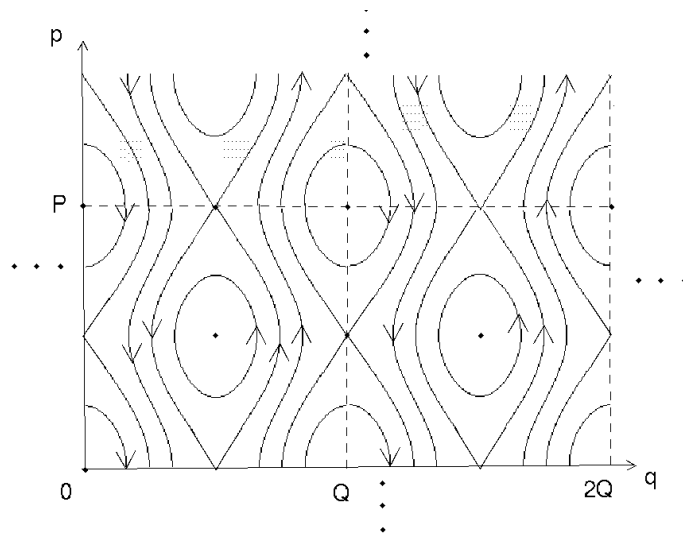


FIG. 1. Trajectories of the Harper model (3).

B. Quantum mechanics on the torus

The Hilbert space of a particle with one-degree of freedom is $L^2(\mathbb{R})$, with the fundamental operators of position \hat{q} and momentum \hat{p} acting on a wave function $\psi(x)$, also noted $|\psi\rangle$.

We now choose a symmetric quantization procedure: to the classical Hamiltonian H , we associate the quantum Hamiltonian:

$$\hat{H} = \sum_{n_1, n_2 \in \mathbb{Z}^2} \frac{1}{2} c_{n_1, n_2} \exp(i2\pi n_1 \frac{\hat{q}}{Q}) \exp(i2\pi n_2 \frac{\hat{p}}{P}) + \text{hermitian conjugate}$$

We denote by \hat{T}_Q [respectively \hat{T}_P] the translation operator by one period. \hat{T}_Q translates by Q a wave function $\psi(x)$ and \hat{T}_P translates its Fourier transform $\hat{\psi}(p)$ by P :

$$\hat{T}_Q \psi(x) = \psi(x - Q) \quad (4)$$

$$\hat{T}_P \hat{\psi}(p) = \hat{\psi}(p - P) \quad (5)$$

We may rewrite equations (4) and (5) as:

$$\hat{T}_Q = \exp(-iQ\hat{p}/\hbar), \quad \hat{T}_P = \exp(iP\hat{q}/\hbar)$$

Quantum mechanically speaking, the periodicity Eq. (1) reads:

$$[\hat{H}, \hat{T}_Q] = [\hat{H}, \hat{T}_P] = 0 \quad (6)$$

To continue, we now have to assume that

$$[\hat{T}_Q, \hat{T}_P] = 0. \quad (7)$$

It is easy to prove that:

$$\hat{T}_Q \hat{T}_P = e^{-i\frac{QP}{\hbar}} \hat{T}_P \hat{T}_Q$$

hence (7) is fulfilled if and only if there exists an integer N such that:

$$N = \frac{QP}{2\pi\hbar} \in \mathbb{N}^* \quad (8)$$

This hypothesis (8) can be regarded as a geometric quantization condition, which states that there is an integer number of Planck cells in the phase space. The semi-classical limit $\hbar \rightarrow 0$ corresponds to the limit $N \rightarrow +\infty$.

Remark 1 For a given periodic Hamiltonian H and a given Planck constant \hbar , the ratio $\frac{PQ}{2\pi\hbar}$ is generically not an integer. But the spectral properties of \hat{H} are in some sense continuous with respect to \hbar , hence we may approximate \hbar by $\hat{\hbar}$ so that $\frac{PQ}{2\pi\hat{\hbar}}$ becomes a rational $\frac{N}{D}$ ([14]). Now to fulfill our hypothesis, we consider H as a periodic hamiltonian with periods $(Q, D \times P)$ (or equivalently $(D \times Q, P)$, many other combinations are possible if D is not a prime number). In the sequel, P and Q denotes periods of H and not necessarily primitive periods of H . From this, we see that it is natural to expect additional translation symmetries of the Hamiltonian inside the (non primitive) periodicity cell and the main results of this work will apply to the $D = 3$ case.

We now assume that Hypothesis (8) is fulfilled.

According to the commutation relations (6) and (7), the Hilbert space $L^2(\mathbb{R})$ may be decomposed as a direct sum of the eigenspaces of the translation operators \hat{T}_Q and \hat{T}_P :

$$L^2(\mathbb{R}) = \int \int H_N(\theta_1, \theta_2) d\theta_1 d\theta_2 \quad (9)$$

$$H_N(\theta_1, \theta_2) = \left\{ |\psi\rangle \quad \text{such that} \quad \begin{cases} \hat{T}_Q |\psi\rangle = \exp(i\theta_1) |\psi\rangle \\ \hat{T}_P |\psi\rangle = \exp(i\theta_2) |\psi\rangle \end{cases} \right\}$$

with $(\theta_1, \theta_2) \in [0, 2\pi]^2$ related to the periodicity of the wave function under translations by an elementary cell. The space of the parameters (θ_1, θ_2) has also the topology of a torus, and will be denoted by T_θ .

The space $H_N(\theta_1, \theta_2)$ is not a subspace of $L^2(\mathbb{R})$, the space of physical states, it is a space of distributions in the x representation, we will see later that it is a subspace of a weighted L^2 space in the Bargmann representation. We will now show that $H_N(\theta_1, \theta_2)$ is finite dimensional. Let $|\psi\rangle \in H_N(\theta_1, \theta_2)$. The Fourier transform of $\psi(x)$ is θ_2 -Floquet-periodic of period P , so $\psi(x)$ is discrete, it is a sum of Dirac distributions supported at points distant from $\frac{h}{P} = \frac{Q}{N}$ from each other. Moreover, $\psi(x)$ is θ_1 -periodic, hence ψ is characterized by the N coefficients at the N Dirac distributions supporting points in the interval $q \in [0, Q]$. Eventually we get:

$$\dim_{\mathcal{T}} H_N(\theta_1, \theta_2) = N$$

Because of Eq. (6) the Hamiltonian \hat{H} is block-diagonal with respect to the decomposition Eq. (9), so we have to consider the spectrum $\sigma(\theta_1, \theta_2)$ of \hat{H} . The operator \hat{H} acts on $H_N(\theta_1, \theta_2)$ as a $N \times N$ hermitian matrix, its spectrum is made of N eigenvalues:

$$\sigma(\theta_1, \theta_2) = \{E_1(\theta_1, \theta_2), \dots, E_N(\theta_1, \theta_2)\}$$

Let ψ_1, \dots, ψ_N be the corresponding eigenfunctions:

$$\hat{H}|\psi_n(\theta_1, \theta_2)\rangle = E_n(\theta_1, \theta_2)|\psi_n(\theta_1, \theta_2)\rangle \quad n = 1, \dots, N$$

For a given level n , as $(\theta_1, \theta_2) \in T_\theta$ are varying, the energy level $E_n(\theta_1, \theta_2)$ form a band, and (assuming that $E_n(\theta_1, \theta_2)$ is never degenerate $\forall \theta$), the eigenvectors $|\psi_n(\theta_1, \theta_2)\rangle$ form a $2D$ surface in the quantum states space. But for a fixed (θ_1, θ_2) , and any $\lambda \in \mathbb{C}$, $\lambda|\psi_n(\theta_1, \theta_2)\rangle$ is also an eigenvector. So the family of eigenvectors for the level n form a complex-line-bundle (of fibre $\cong \mathbb{C} \ni \lambda$) in the projective space of the bundle $H_N \rightarrow T_\theta$. The topology of this line bundle is characterized by an integer $C_n \in \mathbb{Z}$, called the Chern index. Because of the natural Hilbert scalar product on $L^2(\mathbb{R}) = \int \int H_N(\theta_1, \theta_2) d\theta_1 d\theta_2$, which induce the Berry (or Chern) connection ([4], [25]), this topological number is explicitly given by the integral of the Berry (or Chern) curvature ([27]):

$$C_n = \frac{i}{2\pi} \int \int (\langle \partial_{\theta_1} \psi_n(\theta_1, \theta_2) | \partial_{\theta_2} \psi_n(\theta_1, \theta_2) \rangle - \langle \partial_{\theta_2} \psi_n(\theta_1, \theta_2) | \partial_{\theta_1} \psi_n(\theta_1, \theta_2) \rangle) d\theta_1 d\theta_2 \quad (10)$$

This expression has been used intensively for our numerical calculations. Moreover, it can be shown (see e.g. [1], [8]) that:

$$\sum_{n=1}^N C_n = 1 \quad (11)$$

III. HUSIMI AND BARGMANN REPRESENTATION

We have seen previously that the space H_N is not a subspace of $L^2(\mathbb{R})$. For functions belonging to H_N , it will be more useful to introduce a phase space representation of the quantum states, called the Bargmann representation ([28]).

Consider a Quantum state $|\psi\rangle \in L^2(\mathbb{R})$. In order to characterize the localization of $|\psi\rangle$ in the phase space near the point (q, p) , we first construct a Gaussian wave packet $|qp\rangle$ (coherent state) defined in the x -representation by:

$$\langle x | qp \rangle = \left(\frac{1}{\pi \hbar} \right)^{1/4} \exp\left(\frac{i}{\hbar} p x\right) \exp\left(-\frac{(x - q)^2}{2\hbar}\right)$$

The notation $|qp\rangle$ recalls that the coherent state is localized (in the semi-classical limit) at the point (q, p) of the phase space.

The Husimi distribution of a state $|\psi\rangle$ is defined over the phase space by:

$$h_\psi(q, p) = |\langle qp | \psi \rangle|^2$$

and for $\varphi \in L^2(\mathbb{R})$, we have:

$$\int |\varphi(x)|^2 dx = \int \int | \langle qp | \varphi \rangle |^2 \frac{dq dp}{2\pi\hbar} \quad (12)$$

To characterize the functions of $L^2(T^*\mathbb{R})$ which are (q, p) representations of a state, it is more convenient to introduce a complex representation of the phase space $z = \frac{1}{\sqrt{2\hbar}}(q + ip)$. Another (proportional) expression of the coherent state is then:

$$|z \rangle = \exp(za^+) |0 \rangle$$

with $|0 \rangle$ being the fundamental of the harmonic oscillator $H_0 = \hat{q}^2 + \hat{p}^2$, and a^+ being the associated creation operator. Indeed:

$$|qp \rangle = \exp\left(i\frac{qp}{2\hbar} - \frac{q^2 + p^2}{4\hbar}\right) |z \rangle$$

The following antiholomorphic function of z is called the Bargmann distribution of ψ :

$$b_\psi(z) = \langle z | \psi \rangle$$

Clearly, we have

$$h_\psi(q, p) = |b_\psi(z)|^2 e^{-\frac{q^2 + p^2}{2\hbar}},$$

hence the zeroes of the function $h_\psi(q, p)$ are those of the holomorphic function $b_\psi(z)$, which are localized zeroes in the phase space. Moreover, (12) implies that $\psi \in L^2(\mathbb{R})$ if and only if $b_\psi \in L^2(\mathcal{C}, e^{-|z|^2/\hbar})$ and b_ψ is antiholomorphic.

The same definitions can be applied for a state $|\psi \rangle \in H_N(\theta_1, \theta_2)$. The corresponding Bargmann function is a theta-function [19] and the Husimi distribution is bi-periodic in (q, p) , hence is well defined on the Torus T_{qp} . In this representation, H_N is a subspace of $L^2_{loc}(\mathcal{C}, e^{-|z|^2/\hbar})$ (we keep the weight $e^{-|z|^2/\hbar}$ since it is the natural one in the Bargmann representation).

Remark 2 *The Bargmann and Husimi representation of a function of $H_N(\theta_1, \theta_2)$ are characterized by their N zeroes in a given cell T_{qp} up to a multiplicative constant. Since the N zeroes are constrained to have a fixed sum ([19]), we get the right dimension $N - 1 + 1$ for the Hilbert space $H_N(\theta_1, \theta_2)$.*

IV. SEMI-CLASSICAL EXPECTATION OF THE CHERN INDEX

The question is now to guess the value of the Chern index of a given band from classical informations. The first result in this direction is a characterization of the Chern index from the Husimi distribution [18]:

Proposition 3 *If there exists some point $(q, p) \in T_{qp}$ of the phase space, such that*

$$\forall (\theta_1, \theta_2) \in T_\theta, \quad h_{\psi_n(\theta_1, \theta_2)}(q, p) \neq 0$$

then $C_n = 0$.

The proof is quite simple: if $\langle qp | \psi_n(\theta_1, \theta_2) \rangle$ is never zero then we can select an eigenstate $|\psi_n(\theta_1, \theta_2) \rangle$ in each fiber such that $\arg(\langle qp | \psi_n(\theta_1, \theta_2) \rangle) = 0$, giving us a non-vanishing section of the bundle. This section is also a global frame, hence the bundle is trivial: $C_n = 0$.

As a corollary, we get an important semi-classical result about Chern indices:

Proposition 4 *If the energy level $\Sigma_E = \{(q, p) \text{ such that } H(q, p) = E\}$ consists of a single contractible trajectory, then the Chern index of the bands of energy around E are semiclassically zero (more precisely, if we consider a \hbar -parametrized family of energy bands tending to E as \hbar tends to 0, then for \hbar sufficiently small, the Chern index of the energy band must be 0).*

Indeed the WKB construction of quasimodes in phase space ([30], [16], [22]) shows that the Husimi distribution $h_{\psi_n(\theta_1, \theta_2)}(q, p)$ of the eigenstates are highly concentrated and non-vanishing in the vicinity of the trajectory. Thus, taking (q, p) on the classical trajectory and from the proposition 2, we obtain $C_n = 0$.

Hence, to get a non-zero Chern index, we must investigate situations where the energy level Σ_E is not connected or is non-contractible. In this paper, we will study the first situation. The second one is slightly different, but very interesting since it should explain the generic non-zero Chern index arising from Eq. (11).

We need some results about non-zero Chern indices. In fact, for any fixed point (q, p) , the Chern index C_n is the algebraic number of time that a zero of $h_{\psi_n(\theta_1, \theta_2)}(q, p)$ crosses (q, p) [17]:

Proposition 5 Assume that for each $\theta \in T_\theta$, the eigenvalues $E_n(\theta_1, \theta_2)$ are non-degenerate. Let $Z(\theta_1, \theta_2)$ be the set of the non-ordered N zeroes of $h_{\psi_n(\theta_1, \theta_2)}$. Fix a point (q, p) of the phase space. Define:

$$N(q, p) = \{(\theta_1, \theta_2) \in T_\theta \mid (q, p) \in Z(\theta_1, \theta_2)\}$$

Then:

$$C_n = \sum_{(\theta_1, \theta_2) \in N(p, q)} \pm 1 \quad (13)$$

where the sign \pm corresponds to the local orientation of the mapping Z_i at (θ_1, θ_2) , where $Z = \{Z_1, \dots, Z_N\}$ and $Z_i(\theta_1, \theta_2) = (q, p)$.

For example, if the energy level is made of two connected components Γ_1 and Γ_2 , then from the tunnelling effect, the eigenstates $|\psi_n(\theta_1, \theta_2)\rangle$ are a superposition of quasimodes $|\psi_1\rangle$ and $|\psi_2\rangle$ localized on each trajectory. If this superposition is fluctuating enough when (θ_1, θ_2) are varying, then $h_{\psi_n(\theta_1, \theta_2)}(q, p)$ can vanish for every point (q, p) and we expect to get $C_n \neq 0$. In fact this is possible only for special configurations of the two trajectories. This has been investigated in detail in [10], showing that in specific situations, we can observe $C_n = \pm 1$. In the following sections, we will study the (more complicated) case of three contractible trajectories of energy E .

V. GENERIC FAMILY OF HAMILTONIAN $H_{(\gamma_1, \dots, \gamma_P)}$, CHERN INDICES AND DEGENERACIES.

As in [10], Eq. (13) is not so useful to compute analytically the Chern indices of a given Hamiltonian H . The strategy we will adopt is to build a path of Hamiltonians $H(t)$, $t \in [0, 1]$ such that $H(0) = H$ and $H(1)$ has zero Chern indices (for $H(1)$ no tunnelling effect occurs so eigenfunctions are supported by only one connected and contractible trajectory in the phase space, hence Chern indices are zero). Along the path $H(t)$, Chern indices are constant because a continuous application with discrete values is constant. Exception is when a degeneracy occurs between eigenvalues. In this case the Chern index changes by ± 1 . In order to calculate the Chern indices, we are therefore left to compute these degeneracies.

In this section, we will study a generic parametrized Hamiltonian family (in other words, we will consider a submanifold of the space of Hamiltonians), our main interest is to detect eigenvalues degeneracies.

There is an essential property for our investigations ([29]):

Proposition 6 For a generic family of Hermitian matrices, degeneracies between two levels of the spectrum occur with codimension 3.

This means for example that for a generic 3 dimensional family of Hermitian matrices $M(\gamma_1, \gamma_2, \gamma_3)$ the value of $\gamma_1, \gamma_2, \gamma_3$ for which two levels are degenerate, are points in the space of $(\gamma_1, \gamma_2, \gamma_3)$.

Consider now a parametrized family of classical Hamiltonian H_γ on the torus with external parameters $\gamma = (\gamma_1, \dots, \gamma_p)$. The Fourier components $c_{n1, n2}$ of \hat{H} in Eq. (2), the shape and position of each trajectory in the phase space depend on these classical parameters $\gamma_1, \dots, \gamma_p$. On the quantum side, the matrix of the Hamiltonian in a specific base, depends on the classical parameters $\gamma_1, \dots, \gamma_p$ and on the 2 quantum parameters θ_1, θ_2 . Since degeneracies are of codimension three in the space $(\theta_1, \theta_2, \gamma_1, \dots, \gamma_p)$, they are of codimension 1 (hypersurfaces) if we project them onto the space of classical parameters $(\gamma_1, \dots, \gamma_p)$. In fact for each point $(\gamma_1, \dots, \gamma_p)$ not belonging to such a hypersurface, the Chern index of a given band C_n may be calculated with Eq. (10). If we cross a degeneracy hypersurface corresponding to the band n and $n+1$, the value of C_n and C_{n+1} changes respectively by ± 1 and ∓ 1 (because the sum is conserved: cf. [2]). For example, in a one-dimensional space γ , degeneracies appear as points. For a two-dimensional space, we summarize the previous results as:

Proposition 7 In a two dimensional space (γ_1, γ_2) , degeneracies appear as lines bordering different values of the Chern index. The Chern index changes by ± 1 when crossing a line.

In the previous section, we mentioned that these lines occur only if the tunnelling effect occurs. In the next section, we will determine (in the semi-classical limit) the location of these lines when the tunnelling effect occurs between three trajectories in a periodic cell.

VI. DEGENERACIES DUE TO THE TUNNELLING EFFECT BETWEEN THREE TRAJECTORIES OF ENERGY E

In this section, we consider a generic family of periodic Hamiltonians H_γ . We will use local coordinates $\gamma = (\gamma_1, \dots, \gamma_p)$.

We assume that for a given value of E , the intersection of the periodic torus with the energy level Σ_E consists of three contractible trajectories Γ_i (figure 2, p. 7):

$$\Sigma_E \cap T_{qp} = \{(q, p) \in T_{qp} / H(q, p) = E\} = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3$$

We do not assume that E is non-critical since construction of quasimodes along critical trajectories may be done as in [6], [7]. The only characteristic we will use is that the mean distance between energy levels is of order $\hbar/|\ln \hbar|$ for a critical trajectory, whereas it is of order \hbar for a non-critical trajectory.

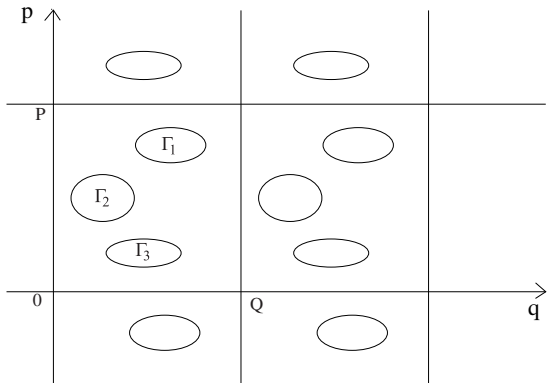


FIG. 2. The energy level E in the phase space.

Our purpose is now to establish under which conditions (shape and locations of the trajectories Γ_i) degeneracies in the spectrum of \hat{H} may occur semi-classically near the energy E . More precisely, we will describe the generic degeneracy lines in the space γ .

A. The tunnelling interaction matrix.

In this section, we construct a basis of $H_N(\theta_1, \theta_2)$ and describe the asymptotic of the matrix of the Hamiltonian H in this basis. To have a more precise picture of these asymptotics, we will make assumptions on the respective decays of interaction terms.

For a first reading, one can skip this section and refer to the results mentionned in proposition 8.

Using the ellipticity of $\hat{H} - E$ outside the classical region $H(q, p) = E$, it is easy to prove that the eigenfunctions are of order $O(\hbar^N)$ for all $N \in \mathbb{N}$ (noted $O(\hbar^\infty)$) outside the classical region. This property is in fact sufficient to construct a basis of $H_N(\theta_1, \theta_2)$.

It is easy to modify the Hamiltonian H in a new hamiltonian \tilde{H}_1 such that:

- the energy shell E of \tilde{H}_1 is Γ_1 ,
- $H = \tilde{H}_1$ outside the shaded region, see figure 3, p.8.

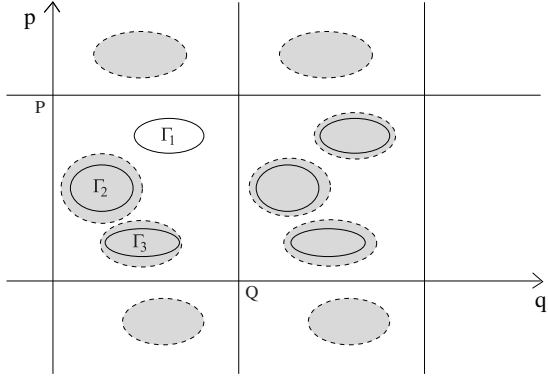


FIG. 3. Modification of H .

Let $|1\rangle$ be an eigenfunction of \tilde{H}_1 corresponding to an eigenvalue $\tilde{E}_1(h)$ such that $\tilde{E}_1(h) \rightarrow E$ as $h \rightarrow 0$. Then $(\hat{H} - \tilde{E}_1)|1\rangle = (\hat{H} - \tilde{H}_1)|1\rangle$. In the last expression, the operator is microlocally supported in the shaded region where $|1\rangle$ is not. Hence:

$$(\hat{H} - \tilde{E}_1)|1\rangle = O(h^\infty)$$

The same construction applies for the trajectories Γ_2 and Γ_3 and we get the functions $|2\rangle$ and $|3\rangle$ microlocally supported on Γ_2 and Γ_3 respectively. In the sequel, we will denote by r the greatest of the quantities $|(\hat{H} - \tilde{E}_i)|i\rangle|$ ($i = 1, 2, 3$).

From $|1\rangle$, $|2\rangle$ and $|3\rangle$ we construct Floquet-periodic quasimodes:

$$|\varphi_i\rangle = P(\theta_1, \theta_2)|i\rangle \quad \text{for } i = 1, 2, 3 \quad (14)$$

where $P(\theta_1, \theta_2)$ is the operator from $L^2(R)$ to $H_N(\theta_1, \theta_2)$ which makes a given state Floquet-periodic:

$$P(\theta_1, \theta_2) := \sum_{n_1, n_2 \in \mathbb{Z}^2} \exp(-in_1\theta_1 - in_2\theta_2) T_Q^{n_1} T_P^{n_2} \quad (15)$$

Figure 4 p.8 and 5 p.9 shows the microlocal support of $|1\rangle$ and $|\varphi_1\rangle$.

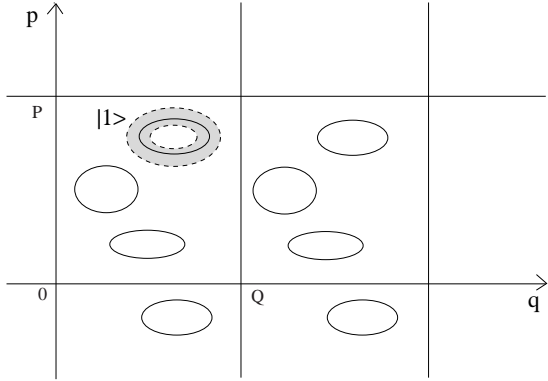


FIG. 4. Microlocal support of the states $|1\rangle$ in the phase space.

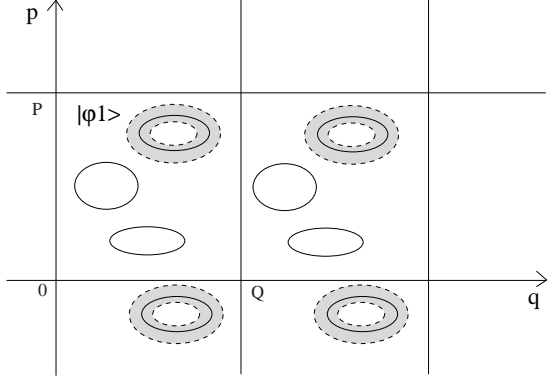


FIG. 5. Microlocal support of the state $|\varphi_1\rangle$ in the phase space.

Suppose that we are in the resonance situation: $\tilde{E}_i(\hbar) - \tilde{E}_j(\hbar) = o(\hbar)$ for $i, j = 1, 2, 3$. Then for $\varepsilon > 0$ sufficiently small the spectrum of \hat{H} in the interval $I = [\tilde{E}_1(\hbar) - \varepsilon\hbar, \tilde{E}_1(\hbar) + \varepsilon\hbar]$ is made of 3 eigenvalues $E_1(\hbar)$, $E_2(\hbar)$ and $E_3(\hbar)$, and if we denote by $\Pi_I(\theta)$ the corresponding spectral projector of $H_N(\theta)$, the spectral space is spanned by:

$$|\psi_i\rangle = \Pi_I(\theta)|\varphi_i\rangle, \quad i = 1, 2, 3.$$

Note that for a critical trajectory the width of the interval must be $\varepsilon\hbar/|\ln \hbar|$.

Let C be the circle of center $\tilde{E}_1(\hbar)$ and radius $\varepsilon\hbar$ in the complex plane. We represent Π_I and identity as:

$$\Pi_I = \frac{1}{2\pi i} \int_C (\hat{H} - z)^{-1} dz, \quad Id = \frac{1}{2\pi i} \int_C (\tilde{E}_1 - z)^{-1} dz \quad Id,$$

and get:

$$\begin{aligned} |\psi_i\rangle - |\varphi_i\rangle &= \frac{1}{2\pi i} \int_C [(\hat{H} - z)^{-1} - (\tilde{E}_1 - z)^{-1}] |\varphi_i\rangle dz \\ &= \frac{1}{2\pi i} \int_C -(\hat{H} - z)^{-1} (\tilde{E}_1 - z)^{-1} (\hat{H} - \tilde{E}_1) |\varphi_i\rangle dz \\ &= O(r/h^2) (= O(h^\infty)) \end{aligned}$$

since $\|(\hat{H} - z)^{-1}\| < K/(\varepsilon\hbar)$ and $|\tilde{E}_1 - z|^{-1} < K/(\varepsilon\hbar)$ for $z \in C$. In the following text, we replace r/h^2 by r , the new r function has decay properties similar to the original one ($r = O(h^\infty)$) and is probably exponentially decaying).

Hence $|\psi_i\rangle$ is microlocalized on Γ_i like $|\varphi_i\rangle$.

The next step is to get an orthonormalized basis from the $(|\psi_i\rangle)_i$. Let

$$n_{ij} = \langle \psi_j | \psi_i \rangle, \quad N = (n_{ij})_{i,j} \quad (16)$$

Since N is positive hermitian, there exists a unique positive hermitian matrix B such that:

$$B^{-2} = N \quad (17)$$

Let $B = (\beta_{ij})_{i,j}$ (with $\beta_{ij} = \overline{\beta_{ji}}$) and:

$$|e_i\rangle = \sum_j \beta_{ij} |\psi_j\rangle \quad (18)$$

We claim that the family $|e_i\rangle$ is orthonormal. Indeed:

$$\begin{aligned} \langle e_i | e_j \rangle &= \sum_{k,l} \overline{\beta_{ik}} \beta_{jl} \langle \psi_k | \psi_l \rangle \\ &= \sum_{k,l} \beta_{jl} n_{lk} \beta_{ki} \\ &= (BNB)_{ji} \\ &= (Id)_{ji} \end{aligned}$$

The tunnelling interacting matrix is the 3×3 Hermitian matrix:

$$A = (\langle e_i | \hat{H} | e_j \rangle)_{ij} \quad (19)$$

The eigenvalues of A are exactly the eigenvalues of \hat{H} which belong to the I interval.

We will now compute the semi-classical asymptotics of a_{ij} . Let:

$$G = (\langle \psi_i | \hat{H} | \psi_j \rangle)_{i,j=1,2,3} \quad (20)$$

From Eq. (18), we get:

$$A = \overline{B} G \overline{B} \quad (21)$$

hence we want to compute asymptotics of B and G .

First we remark that in Eq.(16), we can replace $|\psi\rangle$ by $|\varphi\rangle$, since by Pythagoras theorem:

$$\langle \varphi_i | \varphi_j \rangle = \langle \psi_i | \psi_j \rangle + \langle \varphi_i - \psi_i | \varphi_j - \psi_j \rangle = \langle \psi_i | \psi_j \rangle + O(r^2) \quad (22)$$

Since \hat{H} commutes with Π_I , we get by the same method:

$$\langle \varphi_i | \hat{H} | \varphi_j \rangle = \langle \psi_i | \hat{H} | \psi_j \rangle + \langle \varphi_i - \psi_i | \hat{H} | \varphi_j - \psi_j \rangle = \langle \psi_i | \hat{H} | \psi_j \rangle + O(r^2)$$

We have

$$\langle \varphi_i | \varphi_j \rangle = \delta_{ij} + O(r)$$

Hence:

$$N = Id + O(r), \quad B = Id + O(r) \quad (23)$$

Now, we want to expand the functions $|\varphi_i\rangle$ using (14) and (15) and evaluate the scalar products. From Eq.(20) and (14), we get:

$$\langle \psi_1 | \hat{H} | \psi_1 \rangle = \langle 1 | \hat{H} | 1 \rangle + 2 \sum_{\vec{n} \in D} \text{Re} \left(\exp(-i\vec{n}\vec{\theta}) \langle 1 | \hat{H} | 1_{\vec{n}} \rangle \right) \quad (24)$$

where:

- $\vec{n} = (n_1, n_2)$, $\vec{\theta} = (\theta_1, \theta_2)$,
- $D = \{(\mathbb{Z} \times \mathbb{N}) \setminus (-\mathbb{N} \times \{0\})\}$ is the half plan of \vec{n} ,
- $|1_{\vec{n}}\rangle = T_Q^{n_1} T_P^{n_2} |1\rangle$ is a quasi mode concentrated on the translated trajectory $(\Gamma_1)_{n_1, n_2}$ in the (n_1, n_2) cell of the phase space.

The first term of (24) is $\tilde{E}_1 + O(r^2)$. The term $\langle 1 | \hat{H} | 1_{\vec{n}} \rangle$ is of order $O(r)$ because it corresponds to the tunnelling interaction between the quasimode $|1\rangle$ localized in cell $(0,0)$ and the quasi mode $|1_{\vec{n}}\rangle$ localized in the cell $(n_1, n_2) \neq (0,0)$ (we may need to modify the function r to get this decay: r denotes the strongest tunneling interaction between two components of the energy shell). Hence:

$$\langle \psi_1 | \hat{H} | \psi_1 \rangle = \tilde{E}_1 + O(r)$$

Similar asymptotics hold for the other diagonal terms.

A non-diagonal term of G is e.g.:

$$\langle \psi_1 | \hat{H} | \psi_2 \rangle = \sum_{\vec{n} \in \mathbb{Z}^2} \exp(-i\vec{n}\vec{\theta}) \langle 1 | \hat{H} | 2_{\vec{n}} \rangle \quad (25)$$

And there is generically only one leading term due to the strongest tunnelling interaction between $|1\rangle$ and $|2_{\vec{n}_{12}}\rangle$ (located in the cell \vec{n}_{12} : \vec{n}_{12} may be for example $(0,0)$ or $(0, \pm 1)$ or $(\pm 1, 0)$), of strength

$$\langle 1 | \hat{H} | 2_{\vec{n}_{12}} \rangle = m_{12} \exp(i\varphi_{12})$$

where $m_{12} > 0$ is $O(r)$. This gives:

$$\langle \psi_1 | \hat{H} | \psi_2 \rangle \equiv m_{12} \exp(i(\varphi_{12} - \vec{n}_{12} \vec{\theta}))$$

and similar expressions for others non-diagonal terms. Hence all non-diagonal terms are $O(r)$. If we denote by \tilde{r} the second strongest tunneling interaction, we have

$$\langle \psi_1 | \hat{H} | \psi_2 \rangle = m_{12} \exp(i(\varphi_{12} - n_{12}\theta)) + O(\tilde{r})$$

We assume of course that $\tilde{r} = O(h^\infty)r$.

From $A = \overline{B}G\overline{B}$, $B = N^{-1/2}$ and $N = Id + O(r)$, we get for the diagonal terms of A :

$$a_{ii} = \tilde{E}_i + O(r)$$

and for the non-diagonal terms:

$$a_{ij} = m_{ij} \exp(i(\varphi_{ij} - \vec{n}_{ij} \vec{\theta})) + O(\tilde{r}) \quad (26)$$

To get a more accurate asymptotic of the diagonal terms, we will now study the shifted interaction matrix:

$$\langle e_i | \hat{H} - \tilde{E}_3 | e_j \rangle = \overline{B}(G - \tilde{E}_3 N) \overline{B}$$

We have $G - \tilde{E}_3 N = (\langle \psi_i | \hat{H} - \tilde{E}_3 | \psi_j \rangle)_{ij}$. For the non-diagonal terms, we get similar asymptotics as above (26) with new constants. For simplicity, we will however keep the same notations, since the decays remain of the same order and the phases were not explicit. For the diagonal terms, we get by the same method:

$$(\langle \psi_i | H - \tilde{E}_3 | \psi_i \rangle) = \tilde{E}_i - \tilde{E}_3 + m_{ii} \cos(\varphi_{ii} - n_{ii}\theta) + \dots \quad (27)$$

Since $B = I$ modulo $O(r)$ and $G - \tilde{E}_3 N$ is of order $O(\tilde{r})$, the shifted interaction matrix is $G - \tilde{E}_3 N$ modulo an error of order $O(\tilde{r})$.

In this section we have used the fact that the tunnelling interaction gives terms of order $r = O(h^\infty)$. In fact the reader may replace $O(h^\infty)$ by $O(e^{-S/h})$ which is conjectured to be the right decay order, where S is similar to the Agmon distance between two trajectories (as in the Schrödinger case $H = p^2/2 + V(x)$). See [21], [23] for partial results in this direction).

We summarize the results of this section:

Proposition 8 *Let H be a Hamiltonian and E an energy such that the energy shell $H = E$ is made of three contractible connected components. Let $|1\rangle$, $|2\rangle$, $|3\rangle$ be the quasimodes of \hat{H} localized near one of the three classical trajectories corresponding to eigenvalues $\tilde{E}_1(\hbar) \rightarrow E$, $\tilde{E}_2(\hbar) \rightarrow E$, $\tilde{E}_3(\hbar) \rightarrow E$. Suppose that $\tilde{E}_i(\hbar) - \tilde{E}_j(\hbar) = o(\hbar)$. Then for $\varepsilon > 0$ and $\hbar > 0$ sufficiently small, the spectrum of \hat{H} acting on $H_N(\theta_1, \theta_2)$ in the interval $[\tilde{E}_3(\hbar) - \varepsilon\hbar, \tilde{E}_3(\hbar) + \varepsilon\hbar]$ is made of three eigenvalues.*

We have constructed an orthonormal basis $|e_i\rangle$ spanning the corresponding 3-dimensionnal vector space. Let r be a majorant of the largest tunneling interaction between two different trajectories, and \tilde{r} be a majorant of the second largest tunneling interaction between two wells ($r = O(\hbar^\infty)$ and $\tilde{r} = O(h^\infty r)$). More precisely, we choose i and j in $[1, 3]$, we look at the second strongest interaction between trajectory i and translated of the trajectories j , excluding the 0 translation if $i = j$. r and \tilde{r} are conjectured to be exponentially decreasing with respect to r). Then the matrix of \hat{H} in the basis $|e_i\rangle$ has the following asymptotic:

- The non-diagonal terms are $O(r)$, more precisely:

$$a_{ij} = m_{ij} \exp i(\varphi_{ij} - \vec{n}_{ij} \cdot \vec{\theta}) + O(\tilde{r}), \quad m_{ij} = O(r)$$

- The diagonal terms are given by:

$$a_{ii} = \tilde{E}_i + m_{ii} \cos(\varphi_{ii} - \vec{n}_{ii} \cdot \vec{\theta}) + O(\tilde{r})$$

If we look at the dependency of the interaction matrix with respect to the external parameters γ , it is easy to prove that:

$$d_\gamma a_{ij} = (d_\gamma \tilde{E}_i) \delta_{ij} + O(r)$$

where d_γ denote the differential. The first term is dominant, since the variation of \tilde{E}_i is of order \hbar (or $\hbar/|\ln \hbar|$ for a critical trajectory).

Since we are interested in eigenvalue degeneracies, we may subtract $\tilde{E}_1 I_3$ to the interaction matrix, hence the variation of the shifted interaction matrix with respect to γ is described by the variation of $\tilde{E}_1 - \tilde{E}_3$ and $\tilde{E}_2 - \tilde{E}_3$ with respect to γ up to an error of order r . Hence, we will reduce our parameter space to two parameters γ_1 and γ_2 , and we justify in appendix B that they can be chosen as:

$$\begin{aligned}\gamma_1 &= (\tilde{E}_1 - \tilde{E}_3)/\hbar \\ \gamma_2 &= (\tilde{E}_2 - \tilde{E}_3)/\hbar\end{aligned}\tag{28}$$

(replace \hbar by $\hbar/|\ln \hbar|$ for a critical trajectory).

Moreover, since the error is of order $O(r)$, the degeneracy lines in the parameter space will be of $O(\hbar^\infty)$ size (and conjectured to be of exponentially small size). We will come back to this point more precisely in section VI C.

B. Model of a 3×3 interaction matrix, and computation of its Chern indices.

This paragraph is self-contained. From the previous paragraph, we have to consider a continuous mapping on the torus $T_\theta = [0, 2\pi]^2$ into the 3×3 Hermitian matrices:

$$\mathcal{A} : (\theta_1, \theta_2) \in T_\theta \rightarrow A(\theta_1, \theta_2) = (a_{i,j})_{i,j=1,2,3}$$

where the diagonal terms are:

$$a_{ii} = \tilde{E}_i + m_{ii} \cos(\varphi_{ii} - \vec{n}_{ii} \vec{\theta}) \quad i = 1, 2, 3\tag{29}$$

and the non-diagonal terms are

$$a_{ij} = m_{ij} \exp i(\varphi_{ij} - \vec{n}_{ij} \vec{\theta}) \quad i < j = 1, 2, 3\tag{30}$$

with $\vec{n}_{ij} = (n_{1(ij)}, n_{2(ij)}) \in Z^2$ and $\vec{\theta} = (\theta_1, \theta_2)$. We consider $(m_{ij}, \varphi_{ij}, \vec{n}_{ij})_{i,j=1,2,3}$ as fixed. We will study only the dependance of \mathcal{A} with the parameters $(\tilde{E}_1, \tilde{E}_2, \tilde{E}_3)$.

We recall that $(m_{ij}, \varphi_{ij}, \vec{n}_{ij})$ refer to the tunnelling interaction between the three trajectories $(\Gamma_i)_i, i = 1, 2, 3$ as sketched in figure (6), and that \tilde{E}_i is the energy of the quasimodes on trajectory Γ_i .

If no degeneracy occurs in the spectrum of $A(\theta_1, \theta_2)$ (for all $\vec{\theta} = (\theta_1, \theta_2) \in T_\theta$), each eigenvector family has a well defined Chern index. Precisely, each eigenvector family $(|\psi_n(\vec{\theta})\rangle)_{\vec{\theta}}$ for $n = 1, 2, 3$ is a submanifold of the projective space $P(\mathcal{C}^3)$, homeomorphic to T_θ . The complex line bundle structure of $P(\mathcal{C}^3)$ induces a complex line bundle over this submanifold whose topology is characterized by its Chern index. For specific values of the parameters (codimension 1 in the space of $(\tilde{E}_i)_i$) degeneracies occur and this causes a change of the Chern index. In this paragraph we will compute these Chern indices and the locus of the degeneracies in the space of $(\tilde{E}_i)_i$ for each family of eigenvector $(|\psi_n(\vec{\theta})\rangle)_{\vec{\theta}}$ for $n = 1, 2, 3$. First we remark that subtracting the diagonal matrix $\tilde{E}_3 Id$ to A does not change its eigenvectors, so the only non-trivial external parameters are:

$$\begin{aligned}\gamma_1 &= (\tilde{E}_1 - \tilde{E}_3)/\hbar \\ \gamma_2 &= (\tilde{E}_2 - \tilde{E}_3)/\hbar\end{aligned}\tag{31}$$

The locus of the degeneracies we are looking for are lines in the space (γ_1, γ_2) .

A general property of 3×3 Hermitian matrices, mentioned in the appendix A is that a degeneracy occurs for the matrix A if and only if:

$$\begin{aligned}\Im(a_{12}a_{23}a_{31}) &= 0 \\ a_{11} - a_{22} + \frac{a_{12}a_{23}}{a_{13}} - \frac{a_{21}a_{13}}{a_{23}} &= 0 \\ a_{22} - a_{33} + \frac{a_{13}a_{32}}{a_{12}} - \frac{a_{12}a_{23}}{a_{13}} &= 0\end{aligned}\tag{32}$$

\Im stands for imaginary part. Moreover, the degeneracy is between levels $n = 1, 2$ (respect. $n = 2, 3$) if $\Re(a_{12}a_{23}a_{32}) > 0$ (respect. < 0).

The first equation can be written:

$$\Theta = \arg(a_{12}a_{23}a_{31}) = \varphi_{12} + \varphi_{23} + \varphi_{31} - (\vec{n}_{12} + \vec{n}_{23} + \vec{n}_{31})\vec{\theta} \equiv 0 \quad [\pi] \quad (33)$$

The phase Θ can be seen as the total tunnelling phase for the cycle of trajectories $(\Gamma_1, \Gamma_2, \Gamma_3)$. We want to find solutions in $\vec{\theta}$ of this equation for fixed values of $\varphi_{ij}, \vec{n}_{ij}$. For that purpose, *we assume that $(\vec{n}_{12} + \vec{n}_{23} + \vec{n}_{31}) \neq 0$. This is a generic assumption.* This means that the cycle of trajectories $(\Gamma_1, \Gamma_2, \Gamma_3)$ is not contractible on the torus T_{qp} .

To simplify notations, we will assume that $\vec{n}_{12} = \vec{n}_{23} = 0$, $\vec{n}_{31} = (0, 1)$ and $\vec{n}_{ii} = (1, 0)$. This corresponds to the tunnelling interactions sketched with dashed lines in figure (6). For the tunnelling problem considered in this paper, we think (without proof) that this case is the general one after a suitable lattice transformation in $SL(2, Z)$. But for the self-contained problem of this paragraph, the general case is solved in the appendix C.

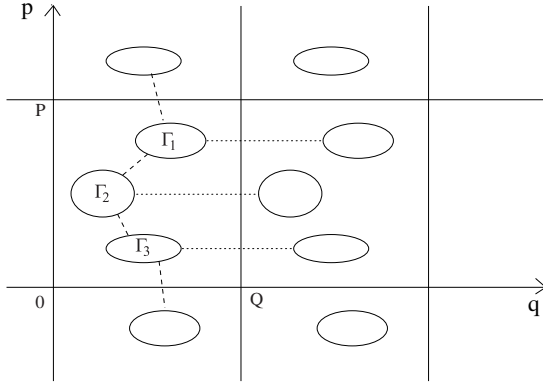


FIG. 6. Example of tunnelling interaction. $\vec{n}_{12} = \vec{n}_{23} = 0$, $\vec{n}_{31} = (0, 1)$ and $\vec{n}_{11} = \vec{n}_{22} = \vec{n}_{33} = (1, 0)$.

Eq. (33) has then two solutions $\theta_2 \equiv \varphi_{12} + \varphi_{23} + \varphi_{31} \quad [\pi]$.

Let

$$s = \exp(i\Theta) = \pm 1.$$

The two-last equations of Eq. (32) give:

$$\tilde{E}_1 - \tilde{E}_3 = sm_{13} \left(\frac{m_{12}}{m_{23}} - \frac{m_{23}}{m_{12}} \right) + m_{33} \cos(\varphi_{33} - \theta_1) - m_{11} \cos(\varphi_{11} - \theta_1) \quad (34)$$

and similarly for $\tilde{E}_2 - \tilde{E}_3$.

Let us remark that:

$$\begin{aligned} A \cos(\theta_1 - \alpha) - B \cos(\theta_1 - \beta) &= (A \cos \alpha - B \cos \beta) \cos \theta_1 + (A \sin \alpha - B \sin \beta) \sin \theta_1 \\ &= D \cos(\theta_1 - \eta) \end{aligned}$$

where:

$$\begin{aligned} D &= \sqrt{A^2 + B^2 - 2AB \cos(\alpha - \beta)}, \\ (\cos \eta, \sin \eta) &= \left(\frac{A \cos \alpha - B \cos \beta}{D}, \frac{A \sin \alpha - B \sin \beta}{D} \right) \end{aligned} \quad (35)$$

So we put:

$$\begin{aligned} K_1 &= \sqrt{m_{11}^2 + m_{33}^2 - 2m_{11}m_{33} \cos \varphi_1} \\ K_2 &= \sqrt{m_{22}^2 + m_{33}^2 - 2m_{22}m_{33} \cos \varphi_2} \end{aligned} \quad (36)$$

where:

$$\varphi_i = \varphi_{ii} - \varphi_{33}$$

and define:

$$Y_1 = m_{13} \left(\frac{m_{12}}{m_{23}} - \frac{m_{23}}{m_{12}} \right) \quad Y_2 = m_{23} \left(\frac{m_{12}}{m_{13}} - \frac{m_{13}}{m_{12}} \right)$$

From (34) and (31), the degeneracy lines in the space (γ_1, γ_2) are the following $t \in \mathbb{R}$ parametrized curves ($s = \pm 1$):

$$\begin{aligned} \gamma_1(t) &= (K_1 \cos(t - \eta) - sY_1)/\hbar \\ \gamma_2(t) &= (K_2 \cos(t) - sY_2)/\hbar \end{aligned} \quad (37)$$

where $s = \pm 1$, $t = \theta_1 - \eta_2$, $\eta = \eta_3 - \eta_2$ and the angles η_2 and η_3 may be computed using (35).

As t describes $[0, 2\pi]$, $(\gamma_1(t), \gamma_2(t))$ describes two translated ellipses of axes parallel to $\gamma_1 = \pm \gamma_2$, one for each $s \in \{-1, 1\}$. $s = 1$ (respect. $s = -1$) gives the degeneracy line between levels $n = 1, 2$ (respect. levels $n = 2, 3$). See figure (7). These two ellipses may intersect, but they don't really intersect in the whole space $(\theta_1, \theta_2, \gamma_1, \gamma_2)$ because they correspond to two different values of θ_2 .

Outside the ellipses, the Chern indices are zero. This is because, when $\gamma_1, \gamma_2 \rightarrow \infty$ the A matrix goes to a diagonal matrix with trivial eigenvectors. Crossing a degeneracy line changes a Chern index change by ± 1 . It can be shown that the value ± 1 is related to the orientation relatively to the orientation of the parametrized ellipse. From this, we deduce the values of the Chern indices in figure (7).

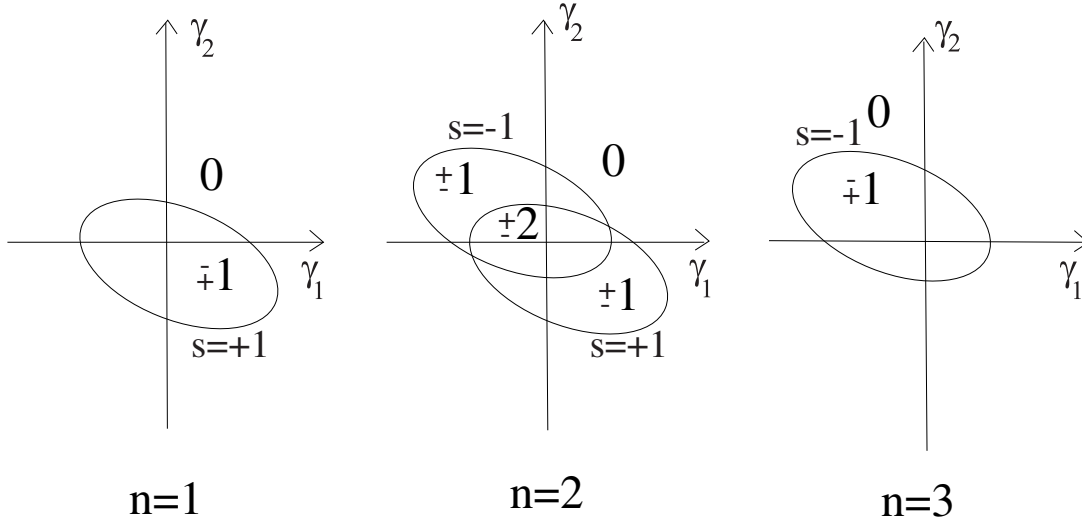


FIG. 7. Degeneracies lines and value of Chern indices from Eq.(37).

C. The degeneracy lines are ellipses.

We are now ready to present the final result. Consider a generic two-dimensional submanifold of the manifold of classical Hamiltonian H_γ (γ are coordinates on this manifold, and can be viewed as external parameters of the Hamiltonian). We have obtained that in this space, degeneracy lines are two ellipses (one for each pair of levels (1, 2) and (2, 3)).

Note that it make sense to state that the shape of the curves are ellipse even if the H_γ -space is a manifold. This is because the ellipse are exponentially small, and thus live in the tangent space.

More precisely, there exist a coordinate system (γ_1, γ_2) (i.e. a special parametrization of the Hamiltonian) for which the two ellipses are given by Eq. (37). The width of the ellipses are given by the coefficients K_1, K_2 , whereas the position of the centers are given by coefficients sY_1, sY_2 , $s = \pm 1$.

It is obvious from Eq. (36) that K_1, K_2 are exponentially small in the semi-classical limit. But this is true also for Y_1, Y_2 . This is shown at the beginning of the appendix (B).

We have then two different generic situations in the semi-classical limit:

1. case: the non-diagonal terms Y_1, Y_2 are exponentially small with respect to the diagonal terms K_1, K_2 . The two ellipses are identical, see figure 8 p. 15. At the origin, the three bands of energy will have Chern indices of $(\mp 1, \pm 2, \mp 1)$. Outside the ellipse, the Chern indices are $(0, 0, 0)$. Note that in the (γ_1, γ_2) parameter space, the ellipse are exponentially small and exponentially flat because K_1 is exponentially small compare to K_2 (or the inverse).

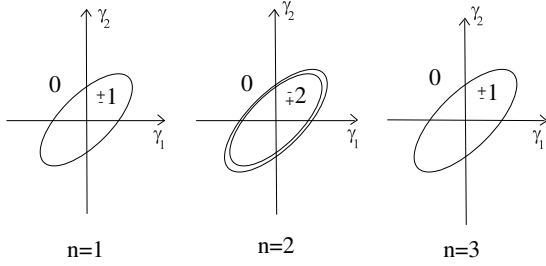


FIG. 8. Degeneracies lines and value of Chern indices in case 1.

2. case: the diagonal terms K_1, K_2 are exponentially small with respect to the non-diagonal ones Y_1, Y_2 . See figure 9, p. 15. At the scale Y_i of the distance between the two center, the degeneracy lines collapse to 2 single points as \hbar tends to 0. Individually these lines are still elliptical with respect to their own scale K_i .

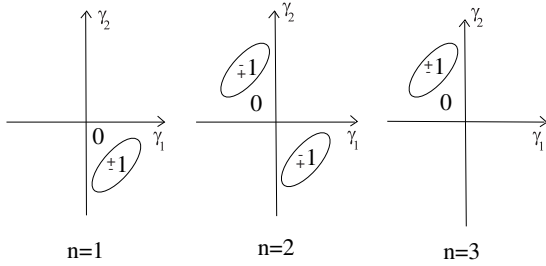


FIG. 9. Degeneracies lines and value of Chern indices in case 2.

The non-generic intermediate case occurs when the diagonal terms K_i and non-diagonal terms Y_i are of the same order. Hence the degeneracies are two ellipses ($s = \pm 1$) with symmetric centers. These two ellipses may intersect. Corrections to the leading behaviour in the semi-classical limit can modify the shape and sizes of the ellipses, see the numerical section.

We now discuss the special translation-symmetric case corresponding to the first calculation of Chern indices done by Thouless and al. [27]. For example, take $H(q, p)$ from Eq. (39) with $b = \gamma_1 = \gamma_2 = 0$. See also remark 1. We construct $|2\rangle = \hat{T}_{P/3}|1\rangle$ and $|3\rangle = \hat{T}_{P/3}|2\rangle$ by translation by $P/3$ in the momentum direction. Applying the relation $T_{P/3}T_Q = e^{2i\pi N/3}T_Q T_{P/3}$ we get:

$$\varphi_2 = \varphi_1/2 = -\varphi_1 = -\frac{2\pi N}{3} \quad (38)$$

Since the non-diagonal m_{ij} are equal, so we are in the first case (double ellipse centered at the origin of figure 8). Assuming that 3 doesn't divide N then we get $K_1 = K_2$ and the precise shape of the ellipse:

$$\gamma_1 = \frac{K}{\hbar} \cos(t), \quad \gamma_2 = \frac{K}{\hbar} \cos(t \pm \frac{2\pi}{3})$$

We conclude that we get an ellipse of axes $\gamma_1 = \pm \gamma_2$ and excentricity $\sqrt{2/3}$.

Remark 9 We want to stress that all the results obtained in this section are valid modulo error terms of order $O(r^2)$, where $r = O(\hbar^\infty)$ is the greatest tunnelling interaction between two wells. If one of the previous contributions m_{ij} between two other wells is smaller than r^2 , it is not significant. For example, if we consider an Hamiltonian where wells 2 and 3 are very closed compared to well 1, our method must be modified, although we think that our results Eq. (37) are still qualitatively correct. In this situation, a more convenient approach is to first treat the cluster of wells 2

and 3 and finally consider the interaction between the cluster and well 1. By this approach, we obtain results similar to those described in [10] for the 2-wells problem.

VII. NUMERICAL ILLUSTRATION

More precise informations on how to perform the numerical simulation, and a software will be available on the web address: <http://www-fourier.ujf-grenoble.fr/~parisse> or <http://lpm2c.polycnrs-gre.fr/~faure>

We take the following Hamiltonian on the torus, parametrized by γ_1 and γ_2 :

$$\begin{aligned} H(q, p) = & \cos(2\pi \frac{q}{Q}) + \cos(6\pi \frac{p}{P}) \\ & + 4b \sin(2\pi \frac{q}{Q}) \cos(2\pi \frac{p}{P}) \\ & + ((\gamma_1 - \gamma_2) \cos(2\pi \frac{p}{P}) + ((-\gamma_1 - \gamma_2) \sin(2\pi \frac{p}{P})) \end{aligned} \quad (39)$$

The two terms in the first line are the main part of the Hamiltonian. They create three symmetric wells in the p direction in the lower part of the energy spectrum, see figure (10). The second line breaks this symmetry, by moving the second well to the left when b increases. b can be seen as a perturbation from the translational symmetric case. The coefficients γ_1 and γ_2 in the third line change the depth of wells 1 and 3 respectively. We therefore expect them to act directly on $(\tilde{E}_1 - \tilde{E}_2)$ and $(\tilde{E}_3 - \tilde{E}_2)$ respectively, such that (B1) will be satisfied. In figure (10) it seems clear that the main tunnelling interactions between the wells are those sketched in figure (6) as assumed for the calculations of the previous section.

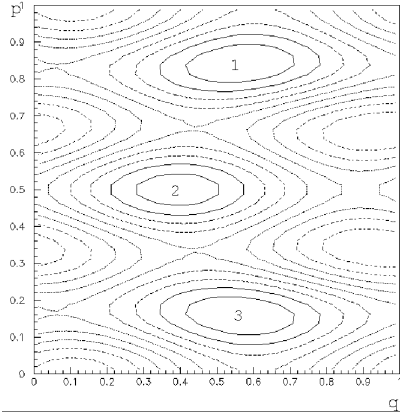


FIG. 10. Contour levels of Hamiltonian (39), with $b = 0.2$ and $\gamma_1 = -\gamma_2 = -0.1$

For the numerical calculations, the Hamiltonian (39) has been diagonalized and formula (10) has been used to obtain the Chern indices C_n . Maps of the Chern indices have been numerically obtained by varying parameters γ_1 and γ_2 .

For $N = 17$ the values of the Chern indices for the first three energy bands $n = 1, 2, 3$ are shown in figure 11.

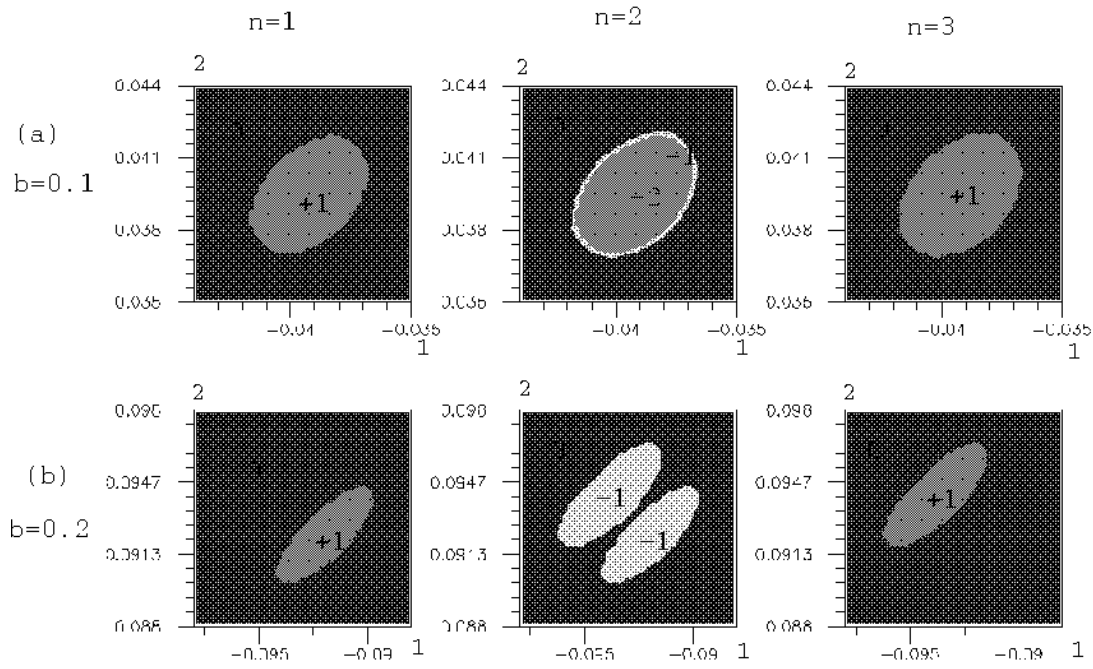


FIG. 11. Chern indices for the first three bands $n = 1, 2, 3$, for $N = 17$. Case (a): The strength of the perturbation is $b = 0.1$. Case (b): The strength of the perturbation is $b = 0.2$.

In case (a), the strength of the perturbation is $b = 0.1$. The two ellipses are degenerated. This is the generic situation depicted in figure (8), and the same generic situation as for the translation-symmetric case with $b = 0$, treated in the previous section. This means that the parameter $b = 0.1$ is small enough to stay in the same generic ensemble.

In case (b), the strength of the perturbation is $b = 0.2$. The two ellipses are separated, as in the second generic situation, sketched in figure (9).

In case (a) and (b), the two ellipses have the same shape, in agreement with the semi-classical results of the previous section.

Figure 12 shows results for a lower value of N , $N = 11$, and for strengths $b = 0.2$ and $b = 0.25$. Here, the generic situations expected in the semi-classical limit $N \rightarrow +\infty$ are less visible. There are still elliptical curves (from a topological point of view), but their position and shapes are affected by non-leading corrections with respect to $N \rightarrow +\infty$.

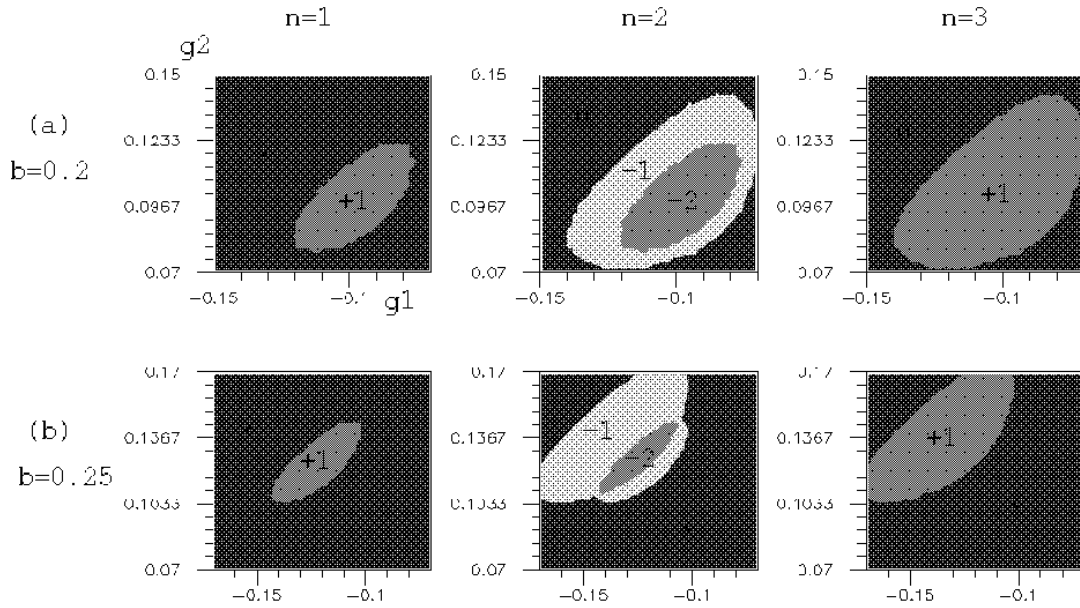


FIG. 12. Chern indices for the first three bands $n = 1, 2, 3$, for $N = 11$. Case (a): The strength of the perturbation is $b = 0.2$. Case (b): The strength of the perturbation is $b = 0.25$.

VIII. CONCLUSION

In this paper, we have shown in which conditions a non-zero Quantum Hall conductivity can occur in the framework of the Harper model, and for the tunnelling between three trajectories in a periodic cell. In this framework, the Hall conductivity is proportional to the topological Chern index. These results were derived semi-classically and give at the same time a description of degeneracies in the spectrum.

Currently, one tries to observe experimental signatures of the Harper spectrum (Landau level substructures) in lateral superlattices with periods of about $100nm$ on GaAs-AlGaAs heterojunctions [12,24]. Our results could therefore have some experimental importance in the future.

The main mathematical gap in this work is that we do not have results about microlocal tunnelling effect (like those obtained by Helffer and Sjöstrand [13] in the Schrödinger case). The main ideas to solve these difficulties are currently majorations of the wave function (A.Martinez [21]), complex paths (estimations of the tunnelling effect by Wilkinson [31,32]), or normal forms (S.Nakamura [23]), but the authors are not aware of a general rigorous result.

Some other related problems could be investigated in the future like:

- numerical localization in the γ -space of the ellipsis (this requires numeric estimations of the tunnelling effect),
- generic interaction between N bands (N -wells tunnelling effect) by a recursive clustering approach,
- the tunnelling effect between non-contractible classical trajectories

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APPENDIX A: EIGENVALUE DEGENERACIES IN 3×3 HERMITIAN MATRICES.

In the text, we use the following result of linear algebra that we have not found in the literature:

Theorem 10 *Let A be a 3×3 Hermitian matrix:*

$$A = \begin{pmatrix} a & \delta & \gamma \\ \bar{\delta} & b & \varepsilon \\ \bar{\gamma} & \bar{\varepsilon} & c \end{pmatrix}$$

where a, b, c are real numbers and $\gamma, \delta, \varepsilon$ are non-zero complex numbers.

Then A has a eigenvalue λ with multiplicity at least 2 if and only if:

$$a - \frac{\bar{\delta}\gamma}{\varepsilon} = b - \frac{\delta\varepsilon}{\gamma} = c - \frac{\gamma\bar{\varepsilon}}{\delta} = \lambda \in \mathbb{R}$$

(this is a system of 3 real equations). The third eigenvalue is $\lambda' = \text{tr}(A) - 2\lambda$ and the spectrum is $(\lambda, \lambda, \lambda')$ with $\lambda' > \lambda$ iff $\Re(\delta\varepsilon\bar{\gamma}) > 0$.

Proof

Let us recall that a hermitian matrix has real eigenvalues and is diagonalizable. Then A has an eigenvalue λ with multiplicity 2 or 3 if and only if its minimal polynomial has degree 2 or 1. The matrix A^2 is then a linear combination of I and A . We have:

$$A^2 = \begin{pmatrix} a^2 + |\delta|^2 + |\gamma|^2 & (a+b)\delta + \gamma\bar{\varepsilon} & (a+c)\gamma + \delta\varepsilon \\ * & b^2 + |\varepsilon|^2 + |\delta|^2 & (b+c)\varepsilon + \bar{\delta}\gamma \\ * & * & |\gamma|^2 + |\varepsilon|^2 + c^2 \end{pmatrix}$$

where the stars denote the conjugate of the symmetric coefficients.

The other eigenvalue is $\lambda' = \text{tr}(A) - 2\lambda$, where $\text{tr}(A)$ denotes the trace of the matrix A . Therefore the minimal polynomial is:

$$P(X) = (X - \lambda)(X - \text{tr}(A) + 2\lambda) = X^2 + (\lambda - \text{tr}(A))X - (2\lambda - \text{tr}(A))\lambda$$

hence:

$$A^2 = (\text{tr}(A) - \lambda)A + \lambda(2\lambda - \text{tr}(A))$$

Eventually we get the system:

$$\begin{cases} a^2 + |\delta|^2 + |\gamma|^2 = (\text{tr}(A) - \lambda)a + \lambda(2\lambda - \text{tr}(A)) \\ b^2 + |\delta|^2 + |\varepsilon|^2 = (\text{tr}(A) - \lambda)b + \lambda(2\lambda - \text{tr}(A)) \\ a^2 + |\varepsilon|^2 + |\gamma|^2 = (\text{tr}(A) - \lambda)c + \lambda(2\lambda - \text{tr}(A)) \\ (a+b)\delta + \gamma\bar{\varepsilon} = (\text{tr}(A) - \lambda)\delta \\ (a+c)\gamma + \delta\varepsilon = (\text{tr}(A) - \lambda)\gamma \\ (b+c)\varepsilon + \bar{\delta}\gamma = (\text{tr}(A) - \lambda)\varepsilon \end{cases} \quad (\text{A1})$$

But $\text{tr}(A) = a + b + c$, so the last three equations simplify to:

$$\begin{cases} \gamma\bar{\varepsilon} = (c - \lambda)\delta \\ \delta\varepsilon = (b - \lambda)\gamma \\ \bar{\delta}\gamma = (a - \lambda)\varepsilon \end{cases}$$

When δ, γ , and ε are non-zero, we verify that these three last equations imply the first three of system Eq. (A1). Indeed by multiplying two with two, we obtain:

$$\begin{cases} |\varepsilon|^2 = (b - \lambda)(c - \lambda) \\ |\delta|^2 = (a - \lambda)(b - \lambda) \\ |\gamma|^2 = (a - \lambda)(c - \lambda) \end{cases}.$$

The spectrum is $(\lambda, \lambda, \lambda')$ iff $3\lambda < \text{tr}(A)$. This gives $\Re(\delta\varepsilon\bar{\gamma}) > 0$.

APPENDIX B: INFLUENCE OF THE EXTERNAL PARAMETERS

In this appendix, we show that generically, only two external parameters γ_1, γ_2 control degeneracies and the Chern indices, as in Eq. (28).

From the generic cyclic assumption made in section VIB, we have the property:

$$\forall i \neq j, i \neq k, j \neq k, \quad m_{ij}m_{jk} \text{ is } O(h^\infty) \text{ with respect to } m_{ik}$$

In the analogous Schrödinger situation, this means that the triangular inequality is strict for the Agmon distance.

Remark 11 *For the Agmon distance, the converse assumption is also generic (wells may be “shaded” by other wells). It is excluded here, because assuming that a well is shaded implies that the cycle of trajectories is contractible.*

For example, if H is symmetric under translation $\hat{T}_{P/3}$, we see that:

$$m_{ij}m_{jk}/m_{ik} = m_{ij} = O(r) = O(h^\infty)$$

Then we get easily that $\tilde{E}_i - \tilde{E}_j$ must be $O(h^\infty)$ in Eq. (34).

More precisely, we want to look at the γ -dependency of the two equations of (34). From the first equation, we define

$$f_1(\gamma, \theta_1) = \frac{1}{\hbar} \left((\tilde{E}_1 - \tilde{E}_3) - \left[sm_{13} \left(\frac{m_{12}}{m_{23}} - \frac{m_{23}}{m_{12}} \right) + m_{33} \cos(\varphi_{33} - \theta_1) - m_{11} \cos(\varphi_{11} - \theta_1) \right] \right)$$

and we define f_2 similarly using the second equation of (34) so that (34) becomes

$$f(\gamma, \theta_1) = 0$$

where

$$f : \begin{cases} \mathbb{R}^p \times [0, 2\pi] & \rightarrow \mathbb{R}^2 \\ (\gamma, \theta) & \rightarrow (f_1, f_2) \end{cases}$$

We see easily that:

$$df = \frac{1}{\hbar} d(\tilde{E}_1 - \tilde{E}_3, \tilde{E}_2 - \tilde{E}_3) + O(h^\infty)$$

If we want to have the simplest possible parametrization of the degeneracies, we have to find 2 parameters such that:

$$J = \partial_2 \text{ parameters} \left(\frac{1}{\hbar} (\tilde{E}_1 - \tilde{E}_3), \frac{1}{\hbar} (\tilde{E}_2 - \tilde{E}_3) \right)$$

is invertible. Hence, we can not take θ_1 as a parameter, and we must take two γ parameters. This means that the degeneracy will not be described by a point on a 1 parameter- γ line but by a line on a 2 parameters- γ plane. We now assume that the parameters γ_1 and γ_2 satisfy the invertibility hypothesis, and more precisely that there exists a constant C such that:

$$|J| \leq C, \quad |J^{-1}| \leq C, \quad \text{with } J = \partial_{\gamma_1, \gamma_2} \left(\frac{1}{\hbar} (\tilde{E}_1 - \tilde{E}_3), \frac{1}{\hbar} (\tilde{E}_2 - \tilde{E}_3) \right) \quad (\text{B1})$$

for γ in an neighborhood of a point γ^0 . In addition, if we suppose that γ^0 is an approximate solution of $f = 0$:

$$f(\gamma^0, \theta_1) = O(h^\infty).$$

we can apply the implicit function theorem with parameter $\hbar, \theta_1, \gamma_3, \dots, \gamma_p$, for $\hbar \in]0, h_0]$ with h_0 sufficiently small such that the rest terms $O(h_0^\infty)$ are smaller than the constants C . We get the existence of an \hbar -independent neighborhood U of $((\gamma^0)_1, (\gamma^0)_2)$ such that for every fixed $(\gamma_3, \dots, \gamma_p)$ in a neighborhood of $((\gamma^0)_3, \dots, (\gamma^0)_p)$ and for every fixed θ_1 , the function $f(\cdot, \gamma_3, \dots, \gamma_p, \theta_1)$ of (γ_1, γ_2) is bijective from U to $f(U)$. Since $f(\gamma^0, \theta_1) = O(h^\infty)$, there exists a unique point $\gamma(\theta_1, \gamma_3, \dots, \gamma_p)$ in U such that $f(\gamma(\theta_1, \gamma_3, \dots, \gamma_p), \theta_1) = 0$ and $|\gamma(\theta_1, \gamma_3, \dots, \gamma_p) - \gamma^0| = O(h^\infty)$.

If we fix $(\gamma_3, \dots, \gamma_p)$ and let θ_1 move, the projection of the point $\gamma(\theta_1, \gamma_3, \dots, \gamma_p)$ in the (γ_1, γ_2) space describes a curve of size $O(h^\infty)$. At that scale, all classical quantities (like tunneling interactions) are constant (with a relative error of order $O(h^\infty)$).

APPENDIX C: MORE GENERAL DEGENERACY CURVES

In this appendix, we solve the general problem raised in section VIB, i.e. we look for the expression of the degeneracy curves in the space X_2, X_3 for any value of $\vec{n}_{ij}, i, j = 1, 2, 3$.

Let us put

$$\vec{N} = \vec{n}_{12} + \vec{n}_{23} + \vec{n}_{31}$$

The first equation of Eq. (32) gives:

$$\Theta = \varphi - \vec{N}\vec{\theta} \equiv 0 \quad [\pi] \quad (\text{C1})$$

with $\varphi = \varphi_{12} + \varphi_{23} + \varphi_{31}$. We put $s = \exp(i\Theta)$. We suppose (see paragraph (VIB)) that

$$\vec{N} \neq \vec{0}$$

There is an unique decomposition of \vec{N} as $\vec{N} = p\vec{M}$ where $p \in \mathbb{N}^*$ is the greatest common divisor of (N_1, N_2) , so (M_1, M_2) are relatively prime. Then Eq. (C1) gives

$$\vec{M}\vec{\theta} = (\varphi + k\pi)/p, \quad k = 1, \dots, 2p \quad (\text{C2})$$

k even (respect. odd) corresponds to $s = +1$ and degeneracy between $n = 1, 2$ (respect. $s = -1$ and degeneracy between $n = 2, 3$).

The last two equations of Eq. (32) give the curves equations as:

$$\gamma_1 = \hbar(-sY_1 + m_{11} \cos(\varphi_{11} - n_{11}\vec{\theta}) - m_{33} \cos(\varphi_{33} - n_{33}\vec{\theta})) \quad (\text{C3})$$

$$\gamma_2 = \hbar(-sY_2 + m_{22} \cos(\varphi_{22} - n_{22}\vec{\theta}) - m_{33} \cos(\varphi_{33} - n_{33}\vec{\theta})) \quad (\text{C4})$$

with γ_i, Y_i defined in paragraph (VIB) and $\vec{\theta}$ is allowed to vary but constrained by Eq. (C2). Because $\vec{M} = (M_1, M_2)$ are relatively prime, there exists \vec{n}_0 from Bézout's theorem such that \vec{M} and \vec{n}_0 form a basis of the \mathbb{Z}^2 lattice, that is $\det[\vec{M}, \vec{n}_0] = 1$. In this basis, we can decompose: $\vec{n}_{ii} = b_i\vec{M} + c_i\vec{n}_0$, with $b_i, c_i \in \mathbb{Z}$ for $i = 1, 2, 3$. This gives

$$\varphi_{ii} - n_{ii}\vec{\theta} = \tau_{i,k} - c_i t$$

with

$$\tau_{i,k} = \varphi_{ii} - b_i\varphi/p - b_i k 2\pi/p, \quad k = 1, \dots, 2p \quad i = 1, 2, 3$$

and a free parameter $t = \vec{n}_0\vec{\theta} \in \mathbb{R}$. The final expression for the degeneracy curves is:

$$\gamma_1(t) = \hbar(-sY_1 + m_{11} \cos(\tau_{1,k} - c_1 t) - m_{33} \cos(\tau_{3,k} - c_3 t)) \quad (\text{C5})$$

$$\gamma_2(t) = \hbar(-sY_2 + m_{22} \cos(\tau_{2,k} - c_2 t) - m_{33} \cos(\tau_{3,k} - c_3 t)) \quad (\text{C6})$$

with $k = 1, \dots, 2p$. This gives $2p$ curves. They can be quite complicated in general. See an example in figure (13). These curves are degenerate if all $c_i = 0$, this means that every \vec{n}_{ii} is proportionnal to \vec{N} . As pointed out in paragraph (VIB), we think that the only possible situation in the Harper model considered in this paper is the ellipse curve, Eq.(37), for which $p = 1, c_1 = c_2 = c_3$.

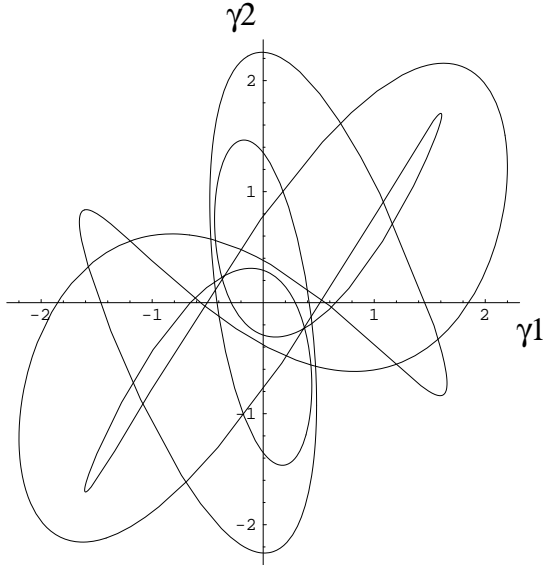


FIG. 13. Parametrized curve $\gamma_1(t) = 1.2 \cos(5t + 1) - \cos(3t)$, $\gamma_2(t) = 1.3 \cos(7t + 0.3) - \cos(3t)$ as an example of the solution Eq.(C5) for a general degeneracy curve.

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